Underworld

a long term geodynamics simulation platform

UNDERWORLD GRID WORKSHOP 2009

Monash University, Caulfield Campus Wednesday 10 June 2009

Presenter: Wendy Mason

Support: Markus Binsteiner & John Mansour











WORKSHOP SPONSORS





Acknowledgments & thanks:

Steve Quenette, Julian Giordani, John Mansour*, Patrick Sunter & Kathleen Humble

Jim McGovern, Darran Carey, Markus Binsteiner*, Sam Morrison & Andy Botting







ABOUT THIS WORKSHOP

- For potential, new and current users of Underworld
- Sample workflow for running Underworld models on computer clusters across the ARCS Grid
 - Grid submission client Grisu graphical user interface
 - pre-installed copies of Underworld-1.2.0 release (no need to install your own copy of Underworld)
 - submit sample models, view & retrieve results
- Brief overview of structure of Underworld model files
- Workshop slides will be posted on Underworld Project website (details at end of workshop)











GETTING HELP

- Underworld user forum / AuScope support: <u>underworld-users@vpac.org</u>
 - AuScope can provide individualised assistance & support with setting up your own models after the workshop
 - to subscribe to and receive emails from this group, go to http://lists.vpac.org/cgi-bin/mailman/listinfo/underworld-users
- Underworld website http://www.underworldproject.org/
 documentation.html
 - guide to getting started on the ARCS Grid
 - Underworld User Manual
 - Component Codex (online & download)
 - Underworld installation guide (basic linux skills required)
- ARCS website & helpdesk http://www.arcs.org.au/support
 - Grisu
 - ARCS Compute Grid & other ARCS Services











ARCS IDP AND SERVICES

- You have already been:
 - ARCS ID

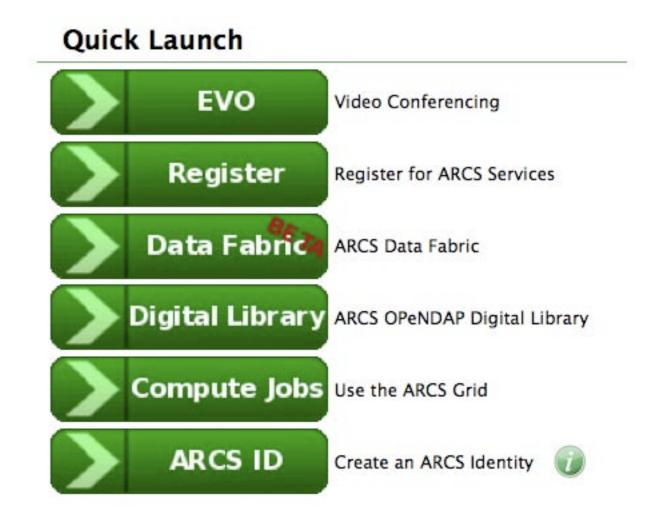
added as a member of the ARCS Identity Provider



registered for ARCS Services

http://www.arcs.org.au/









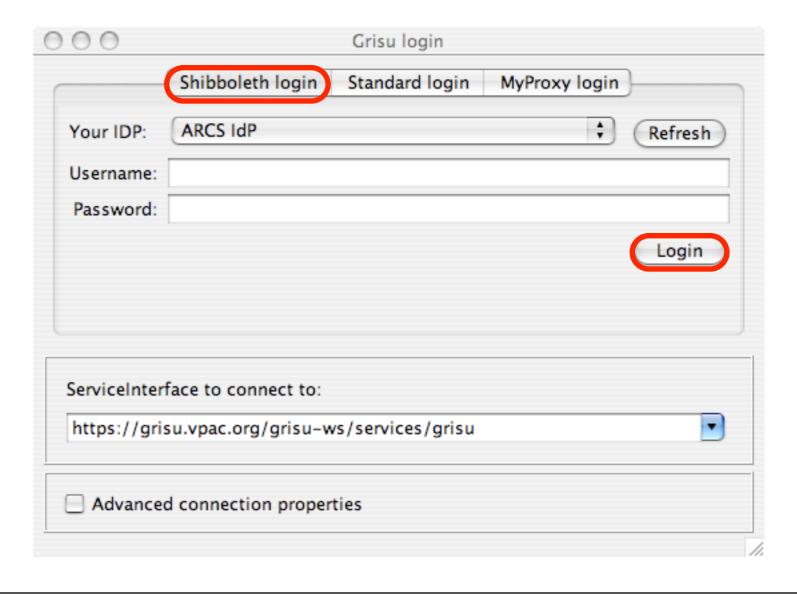






GRISU GRID SUBMISSION CLIENT

- Compute Jobs
- Get Grisu , download grisu.jnlp to your desktop
- Double-click on grisu.jnlp
 - Shibboleth login
 - ARCS IdP
 - enter username& new password
 - Login
- Note: At least Java1.5/5.0 required







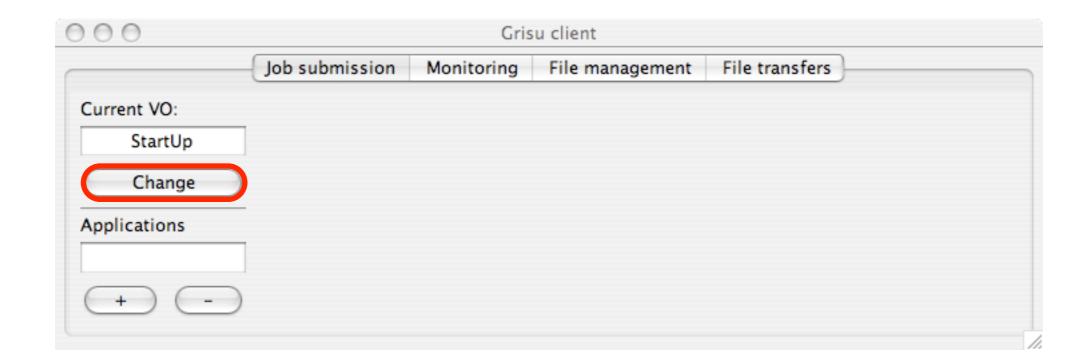






VIRTUAL ORGANISATIONS (VOS)

- Click on the "Change" button and select the Workshop VO
 - StartUp = all new users of ARCS Services (limited access)
 - Workshop = a temporary VO for this workshop (until 19 June)







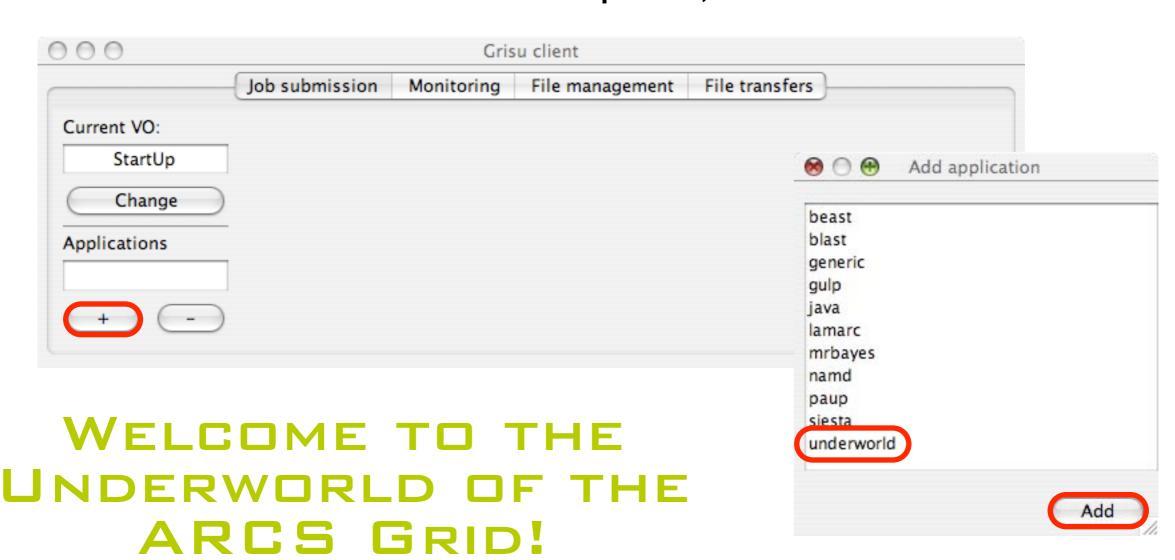






UNDERWORLD TEMPLATE

- Click on "+" button
- Select the "underworld" template, click on "Add" button



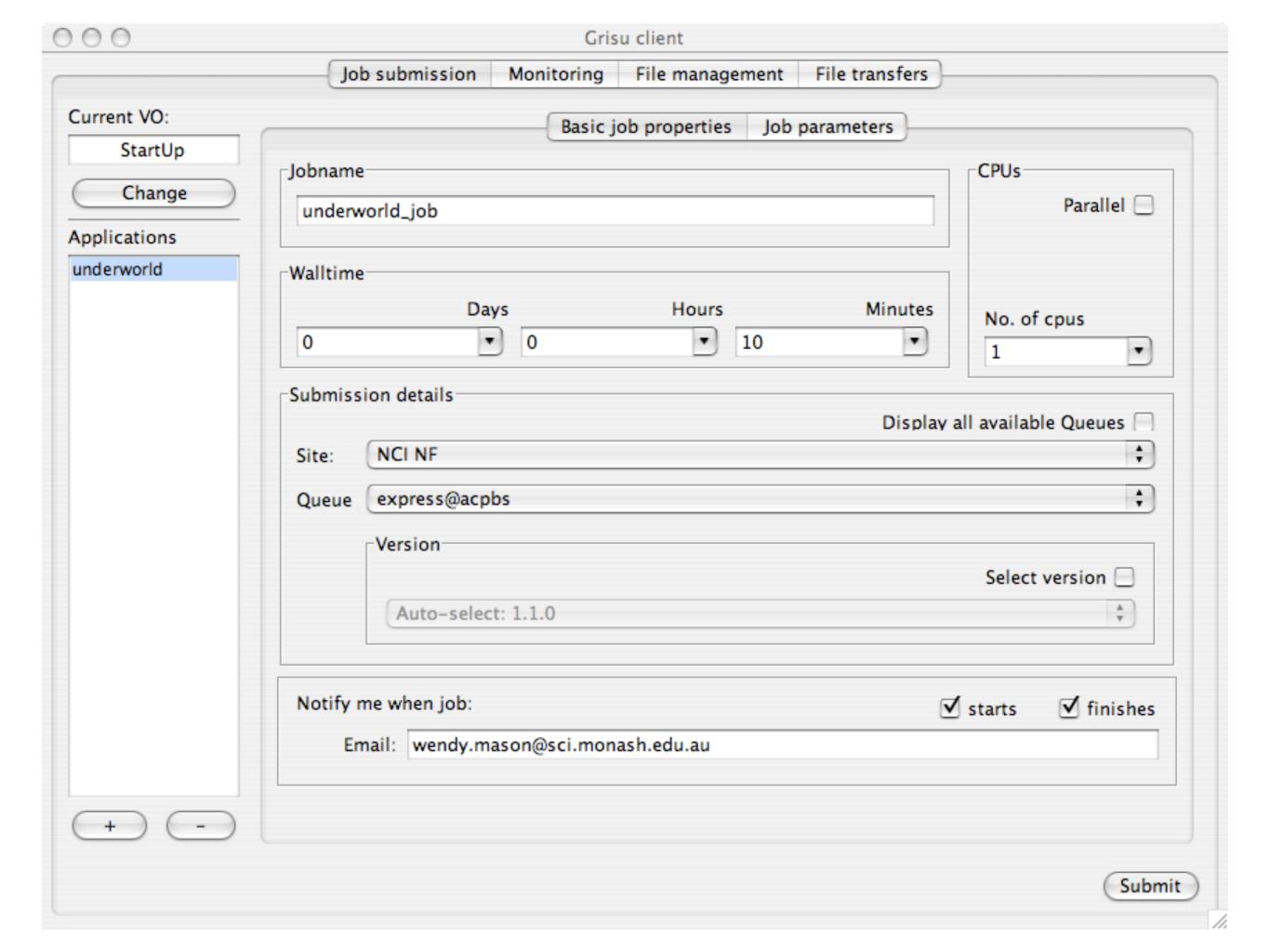












ORKSHOP EXERCISES

- Download files for today's exercise from http://www.underworldproject.org/documentation/ <u>UnderworldGridWorkshop2009.html</u>
- These exercises are modified versions of following four of the several template models that come with Underworld:
 - Extension.xml

- MultiThermalDiffusivity.xml
- RayleighTaylorBenchmark.xml SlabSubduction.xml
- Note that the resolution in today's examples is set very low for the purposes of demonstration
- A full set of template model files for each recent release of Underworld can be downloaded from http://www.underworldproject.org/downloads/











EQUATIONS IN UNDERWORLD

$$\tau_{ij,j}-p_{,i}=\rho(T,C,\ldots)g_i-f_{,i}^{\Delta T}$$

$$u_{i,i} = 0$$

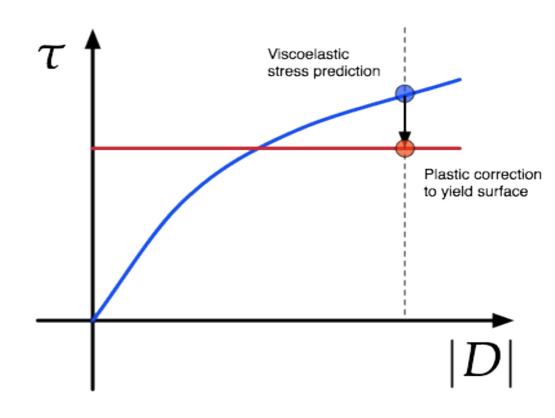
Momentum and Mass conservation

$$\frac{\overset{\triangledown}{\tau}_{ij}}{\mu} + \frac{\tau_{ij}}{\eta} + \alpha \Lambda_{ijkl} \tau_{kl} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}$$

Constitutive rule

$$T_{,t} + u_i T_{,i} = (\kappa T_{,i})_{,i} + Q$$

Energy conservation



Scheme for plastic correction

$$C_{,t}+u_iC_{,i}=0$$

Advection of materials





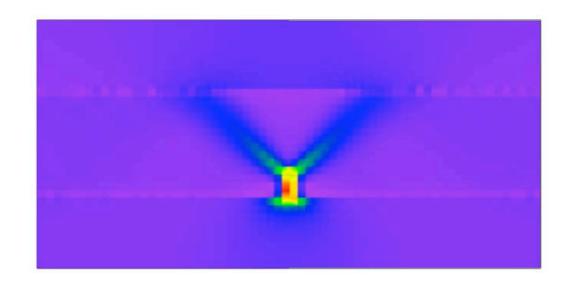


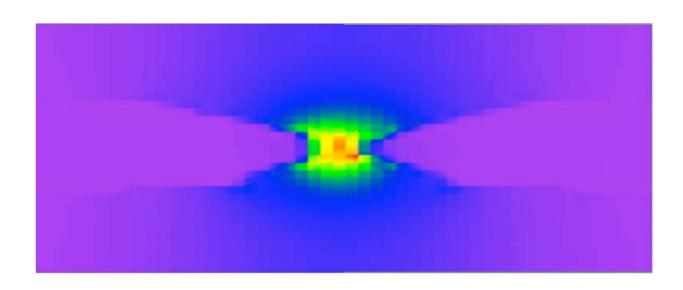




#1: EXTENSION_WORKSHOP.XML

- High viscosity incompressible bar-shaped region which yields according to the VonMises model, in a low viscosity compressible material
- A weak zone is located approximately half-way along the bottom of the region, to facilitate localisation of deformation
- The domain is stretched horizontally, as determined by extensional boundary conditions















BASIC JOB PROPERTIES

- Jobname = name of output directory
- Walltime = maximum length of time job will run
- CPUs = number of processors (at least 2 for mpi jobs)
- Site = organisation(s) to which your VO has access, hosting grid-enabled cluster(s) which have grid-enabled Underworld modules installed
- Queue = grid-enabled cluster(s) at the site & their queue(s)
- Version = grid-enabled Underworld modules installed on the cluster (1.2.0 recommended)
- Notification = receive an email when your job starts & / or finishes; note that Jobname will be shortened in email



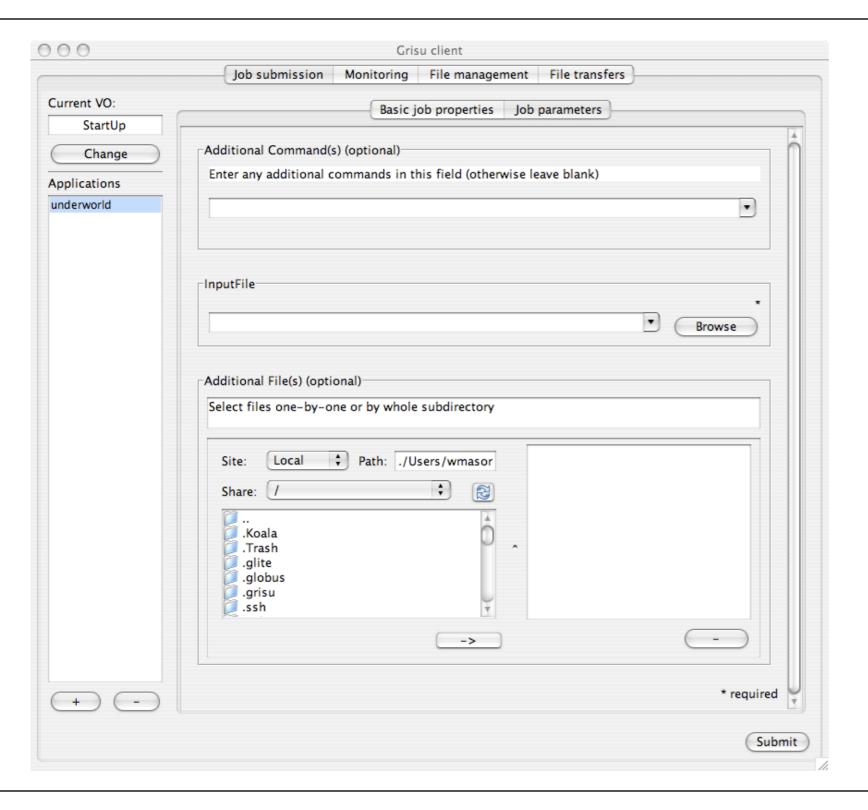








JOB PARAMETERS



Additional Command(s) (optional) = any extra linux command flags (advanced)

InputFile = Underworld model file

Additional File(s)
(optional) =
any other files included /
listed in the model file











- Rayleigh-Taylor convection benchmark, as detailed in:
 - P.E. van Keken et al. A comparison of methods for the modelling of thermochemical convection. Journal of Geophysical Research 102, B10: 22,477 22,495, 1997.
- See Underworld User Manual for:
 - details of benchmark comparison
 - how to create one's own models using this example

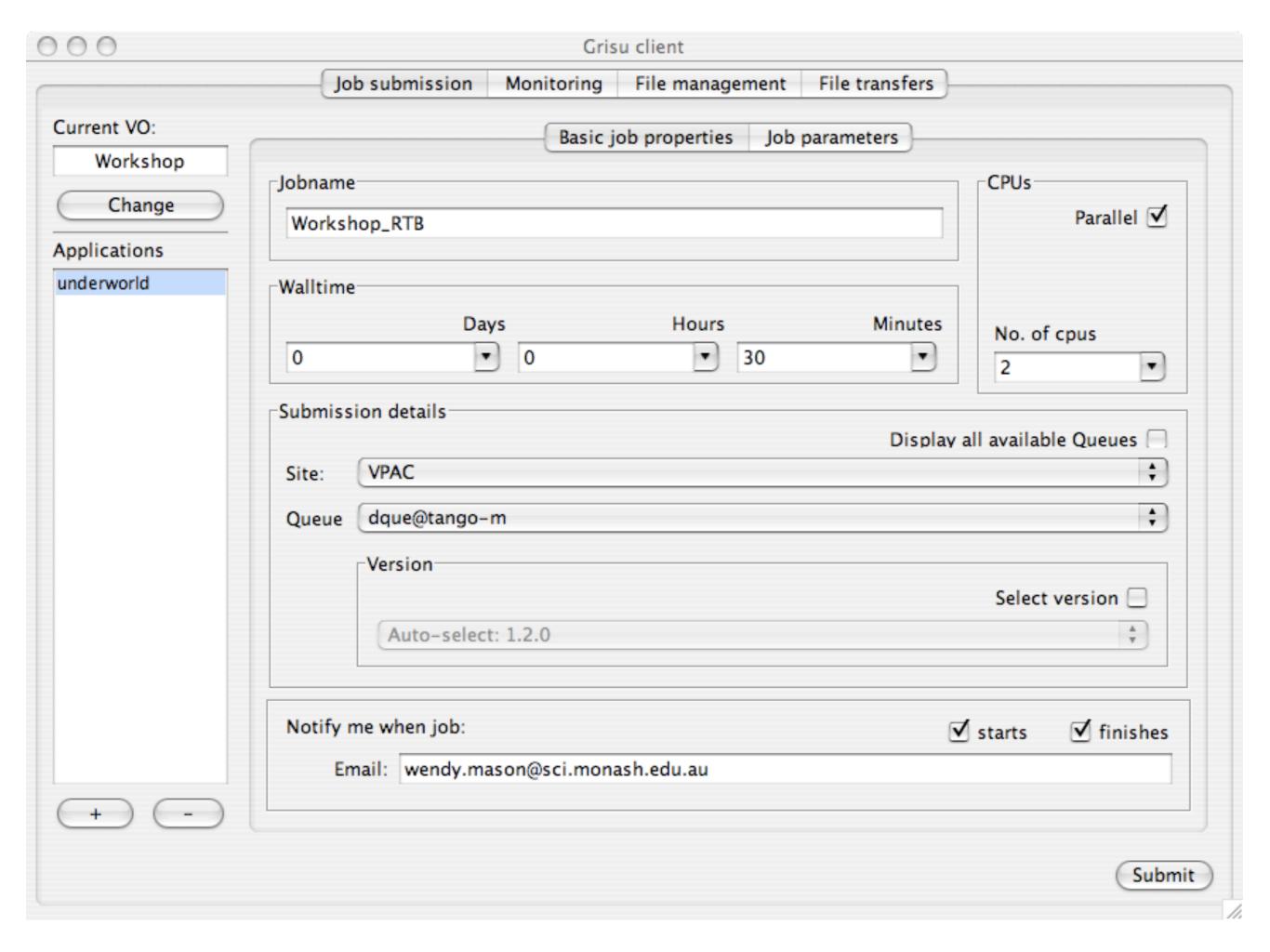


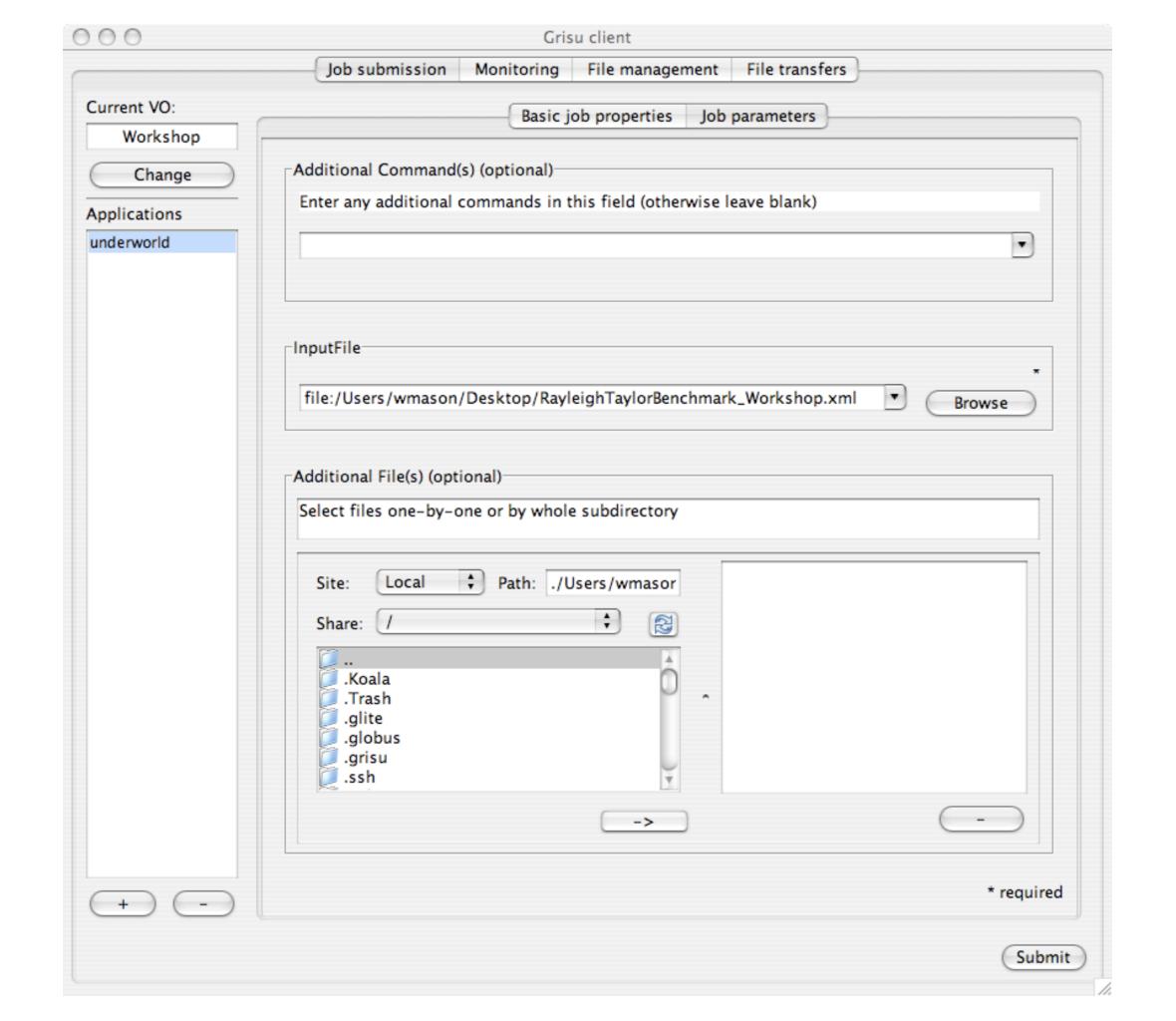


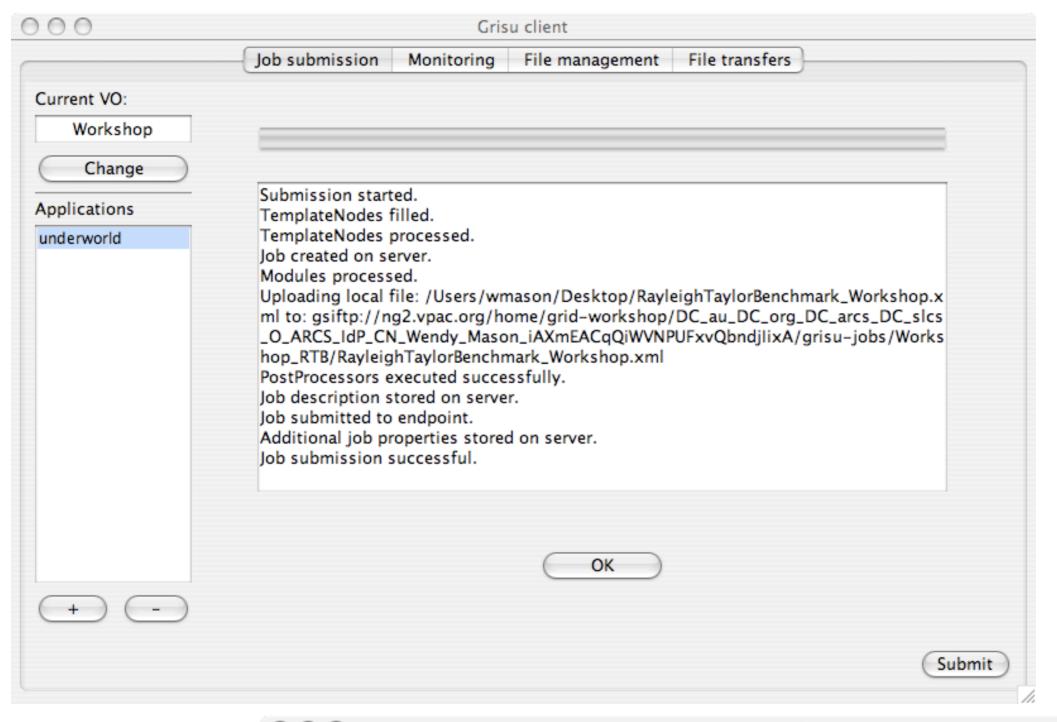


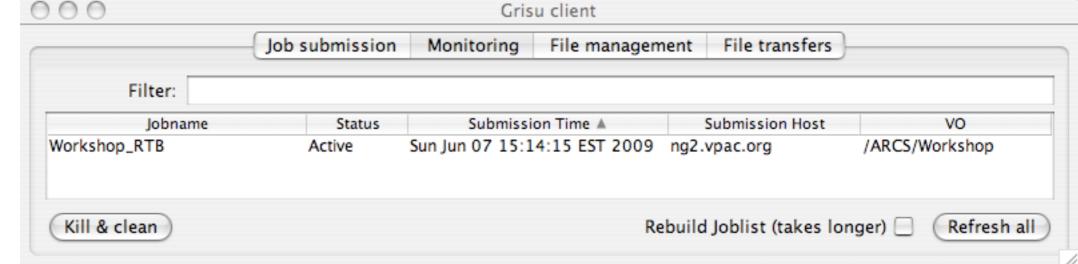






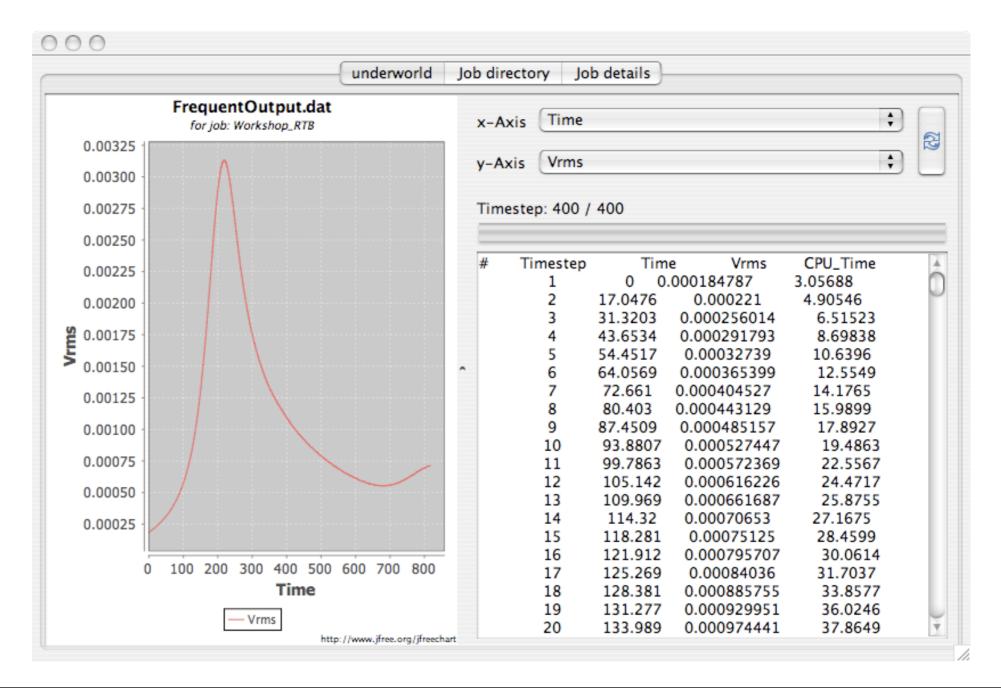






Underworld post-processing panel:

Previews
contents of
FrequentOutput.
dat (data
generated by
output plugins)
& plots a graph
from selected
data columns







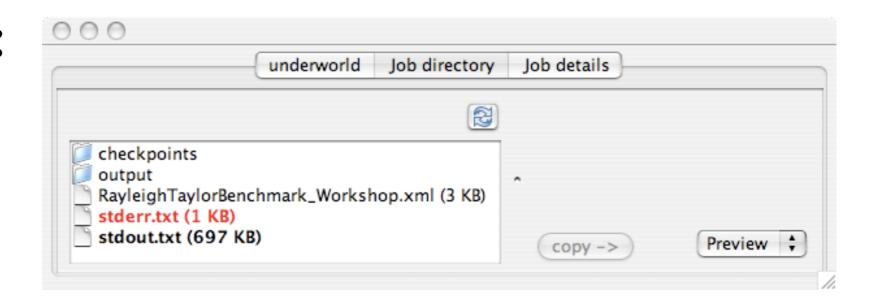






Job directory panel:

- All files staged in
- error (stderr.txt) & output (stdout.txt) files



output subdirectory

```
<param name="outputPath"> ./output/ </param>
```

checkpoints subdirectory (if applicable)

```
<param name="checkpointPath">./checkpoints/ </param>
<param name="checkpointEvery"> 400 </param>
```

- snapshot of fields & swarm
- can be used to restart simulations from previous runs

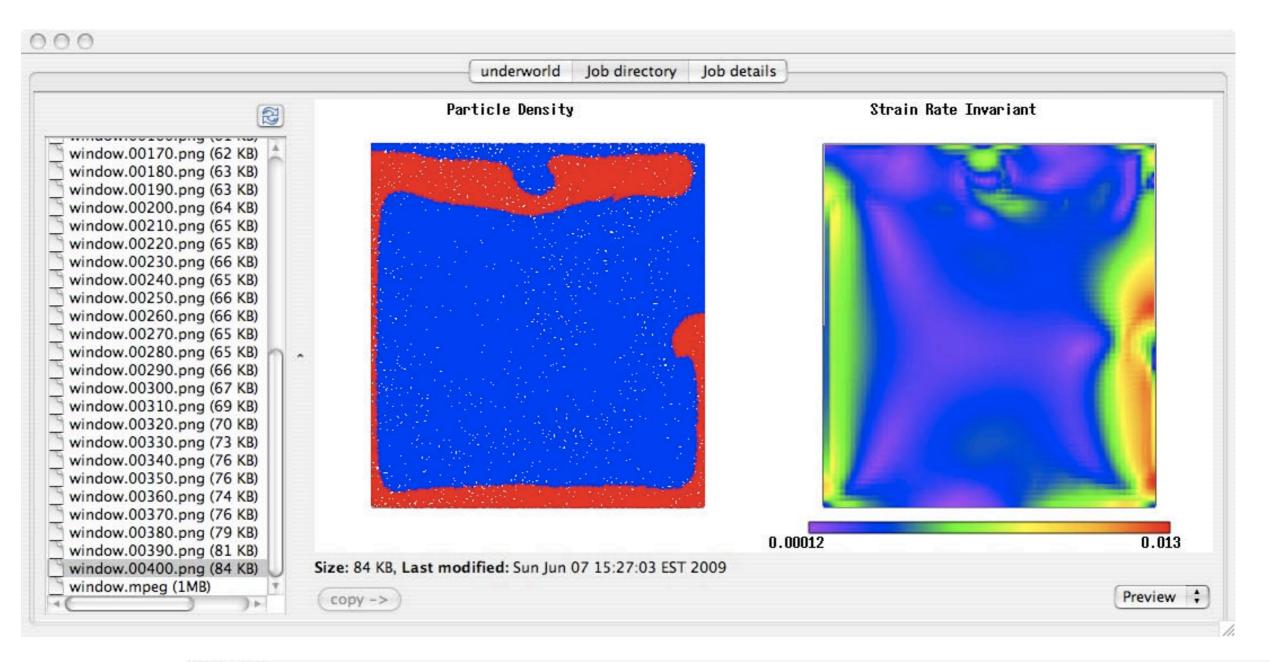


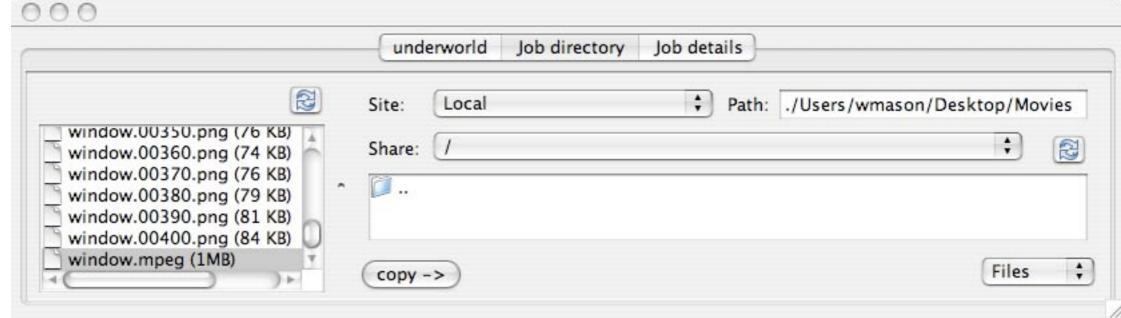




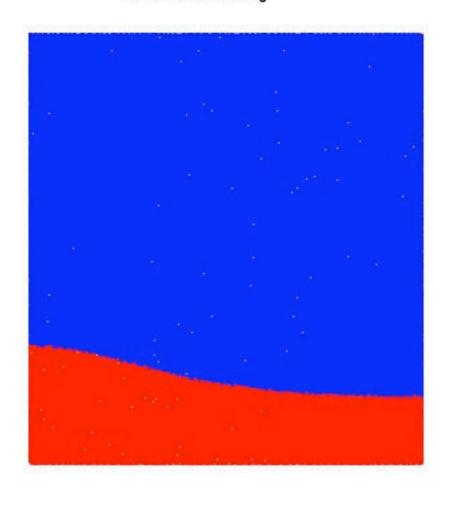




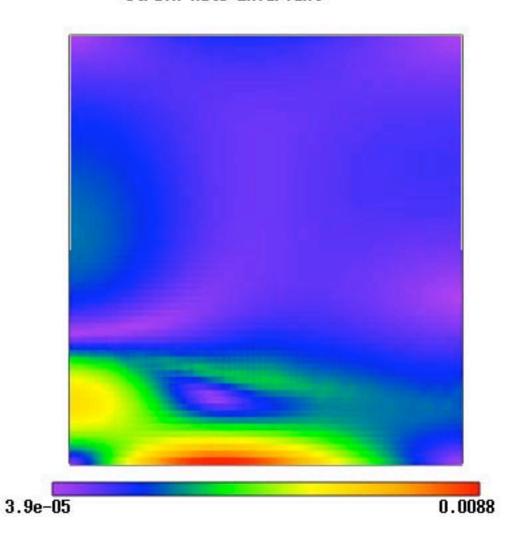




Particle Density



Strain Rate Invariant













- Full time-stamped version of the XML file used (flattened)
- FrequentOutput.dat file
- Underworld comes with the visualisation package gLucifer
 - png image outputs are created by default

```
<param name="maxTimeSteps"> 400 </param>
<param name="dumpEvery"> 10 </param>
```

movie generation (.mpeg) is NOT on by default

```
<include>glucifer/BuildMovies.xml</include>
```

- interactive mode off by default (only available on local machine, not on clusters or the ARCS Grid)
- See Component Codex for other output & checkpoint parameters,
 & output components



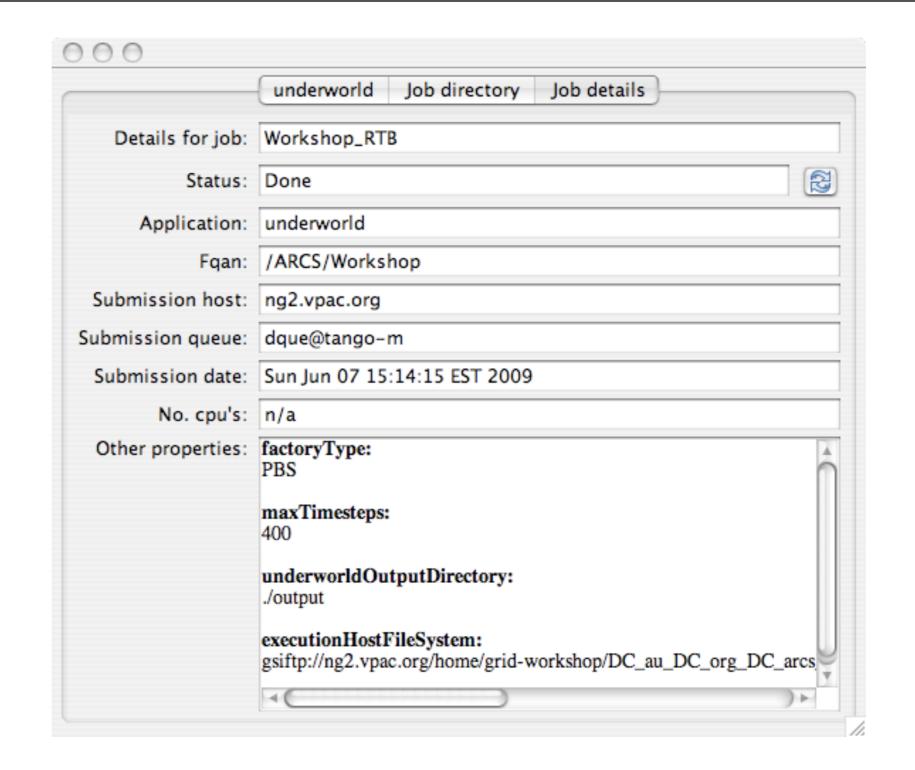








Job details panel:







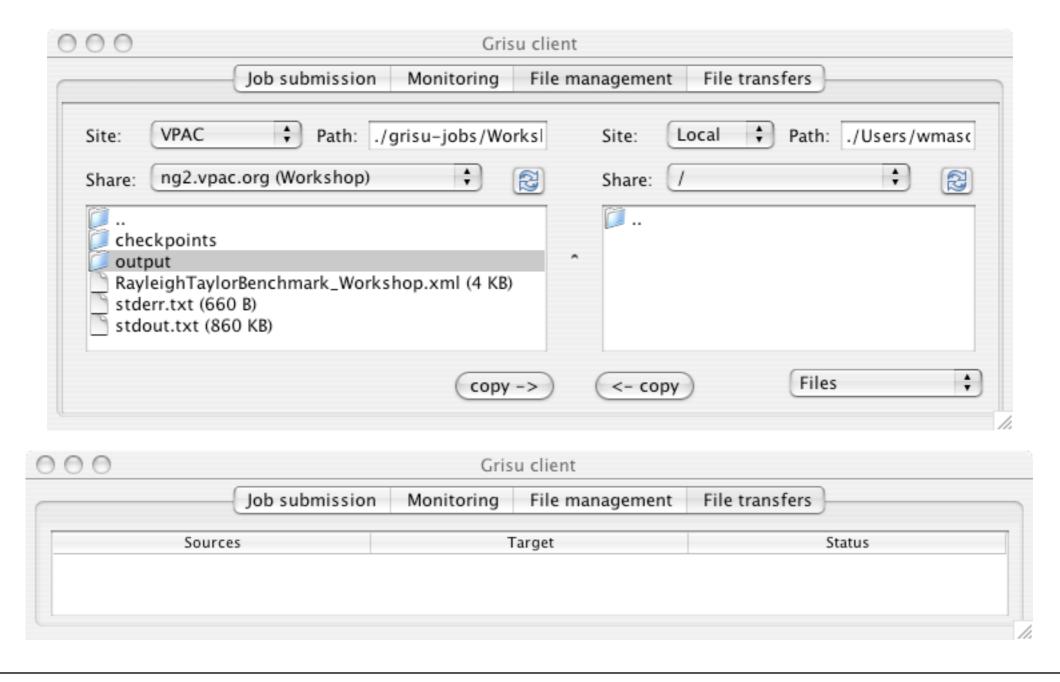






FILE MANAGEMENT / TRANSFERS

Copy to local drive or account on another cluster













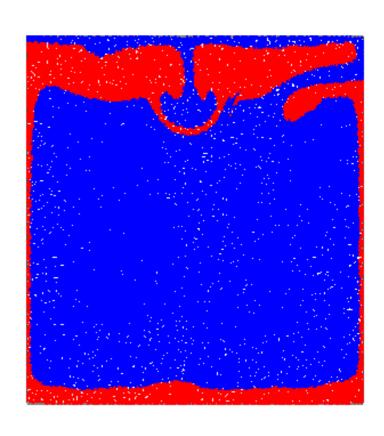
- Now let's restart the previous model from checkpointed files
- Revised output parameters:

```
<param name="maxTimeSteps"> 100 </param>
<param name="dumpEvery"> 10 </param>
<param name="outputPath"> ./output/ </param>
```

Revised checkpoint parameters:

```
<param name="checkpointPath">./checkpoints/ </param>
<param name="restartTimestep"> 400 </param>
```

 Note: checkpoint files generated on one cluster may not work on another architecture



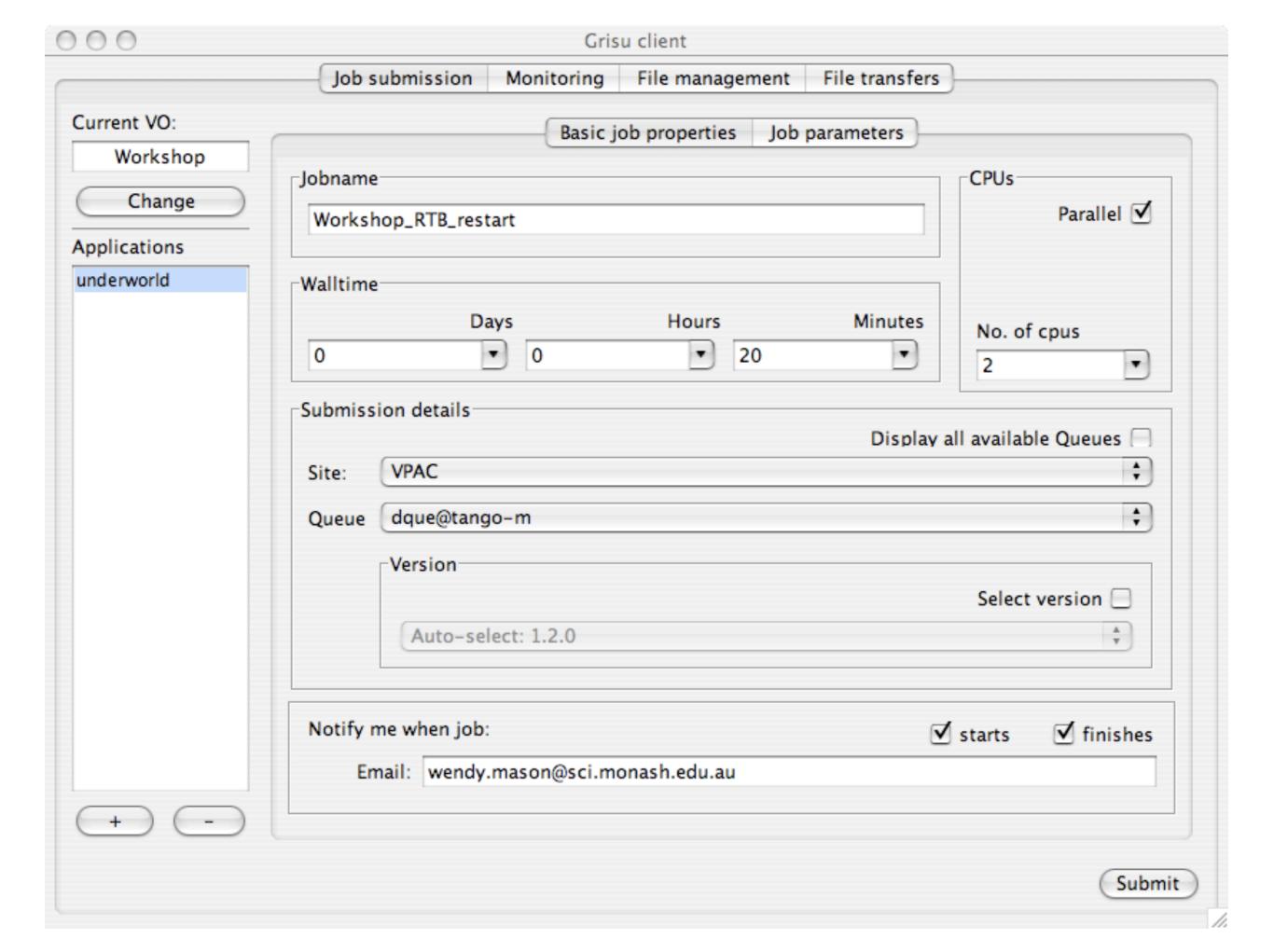


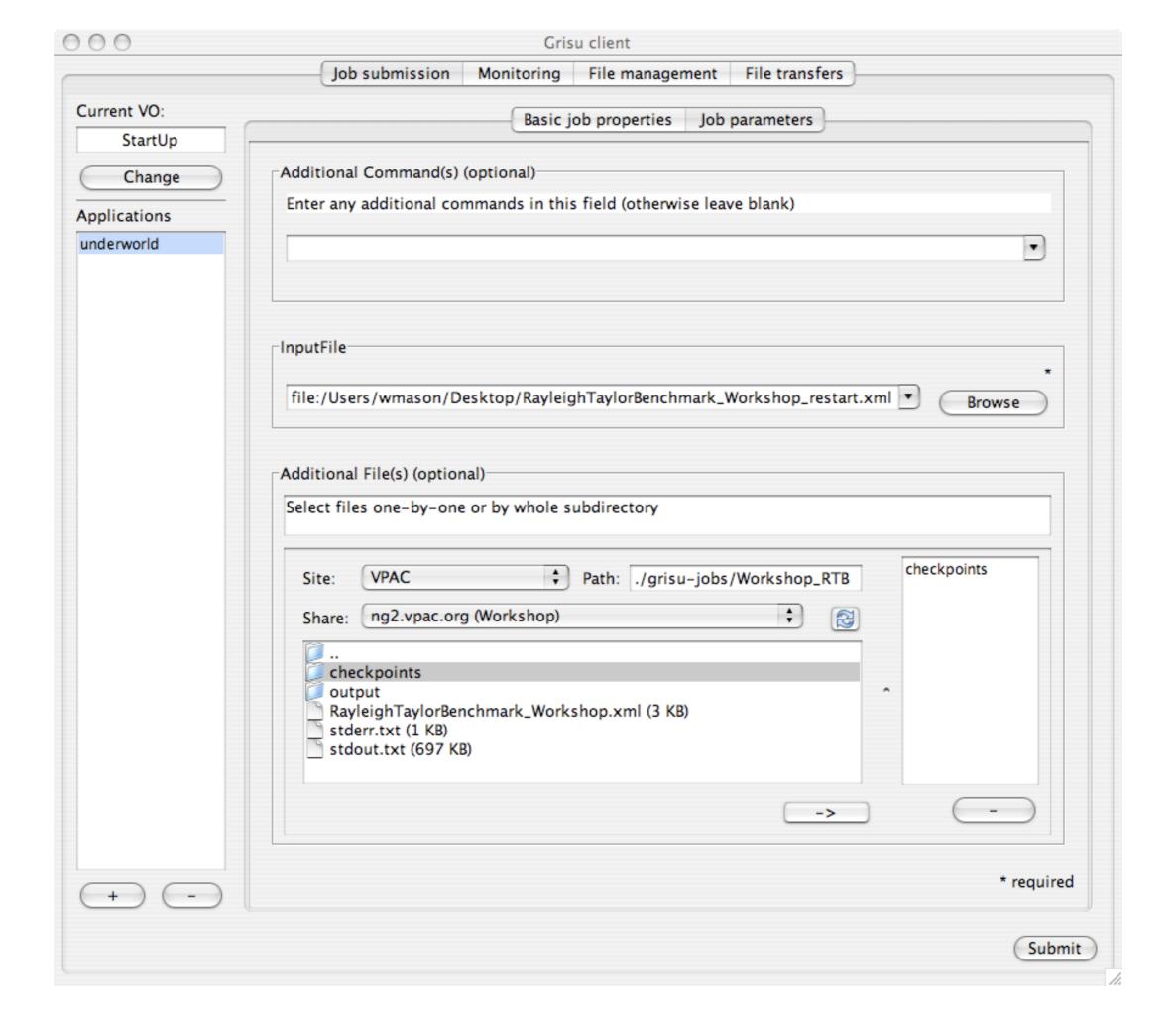












#3: MULTITHERMALDIFFUSIVITY_WORKSHOP.XML

- Contains 3 strips of constant isoviscous material aligned in the y-axis
- Each material has a different diffusivity
- The fluid is driven by a thermal packet which spreads over each material





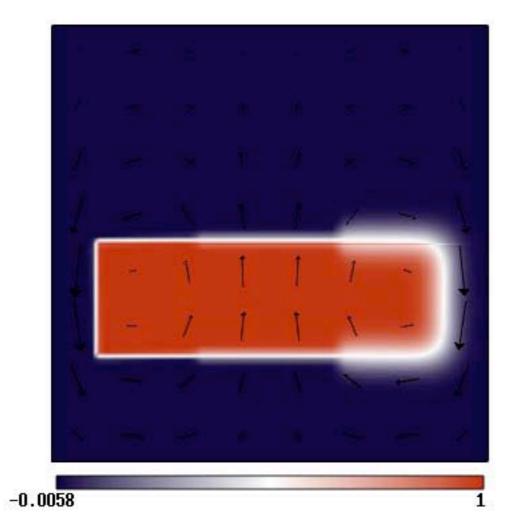




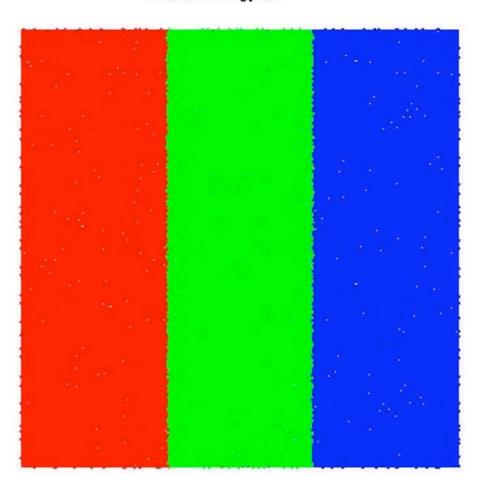


#3: MULTITHERMALDIFFUSIVITY_WORKSHOP.XML

TemperatureField and Velocity Arrows



Particle Types













Underworld Input File Structure

- Underworld is set up to use a hierarchy of XMLs, so your model setup can be split into separate XML files, to be included in your Input File (e.g. different parameter sets)
- All "included" files not part of the Underworld code must be staged in as additional files











All Underworld XML files start & finish with:

```
<StGermainData xmlns="http://www.vpac.org/StGermain/XML_IO_Handler/Jun2003">
...
</StGermainData>
```

You can add comments to your XML files:

```
<!-- comment -->
```

Base application (Underworld/BaseApps/), e.g.

<include>Underworld/BaseApps/RayleighTaylor.xml</include>

Plugins (mostly output plugins), e.g.

```
<list name="plugins" mergeType="merge">
    <!-- Output Plugins -->
        <param>StgFEM_FrequentOutput</param>
        <param>Underworld_Vrms</param>
        <param>StgFEM_CPUTime</param>
</list>
```











Component list:

- Component Codex: http://www.auscope.monash.edu.au/codex-v1.2.0/ work in progress (has been further developed since)
- parent / child relationships between components
- all component lists must use the following format:











- Simulation control parameters, e.g. output, checkpointing
- Geometry & mesh setup, e.g.

Initial & boundary conditions











- Visualisation files / parameters
 - viewports (in Underworld/Viewports/), e.g.

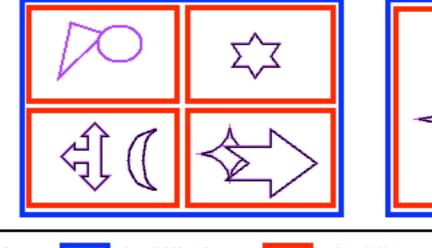
```
<include>Underworld/Viewports/ParticleDensityVP.xml</include>
<include>Underworld/Viewports/StrainRateInvariantVP.xml</include>
```

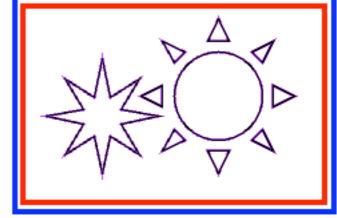
- window(s) containing viewports defined in above files, e.g.

</struct>

 movie generation (not included by default)

<include>glucifer/
BuildMovies.xml</include>





Key:



lucWindow



lucViewport



lucDrawingObject











#4: SLABSUBDUCTION_WORKSHOP.XML

- Slab model as described in:
 - D. R. Stegman et al. Influence of trench width on subduction hinge retreat rates in 3-D models of slab rollback. Geochemistry Geophysics Geosystems 7, Q03012, 2006.
- 3D chemical convection model simulating a falling lithospheric slab
 - dense lithospheric slab with a perturbed tip to initiate subduction
 - viscosity stratification between upper mantle & lower mantle











#4: SLABSUBDUCTION_WORKSHOP.XML

Modified output path:

```
<param name="outputPath">(./)</param>
```

- Note: this is to illustrate that the Underworld post-processing panel will not activate if "FrequentOutput.dat" is not located in a subdirectory defined by this parameter
- Modified visualisation file SlabViewports_Particles_Workshop.xml
- Revisualising from supplied checkpoint files
 - checkpoint files were created on 4 processors
 - revisualising in visual-only mode on 2 processors
 - Note: checkpoint files generated on one cluster may not work on another architecture
- Not generating a movie in this model run

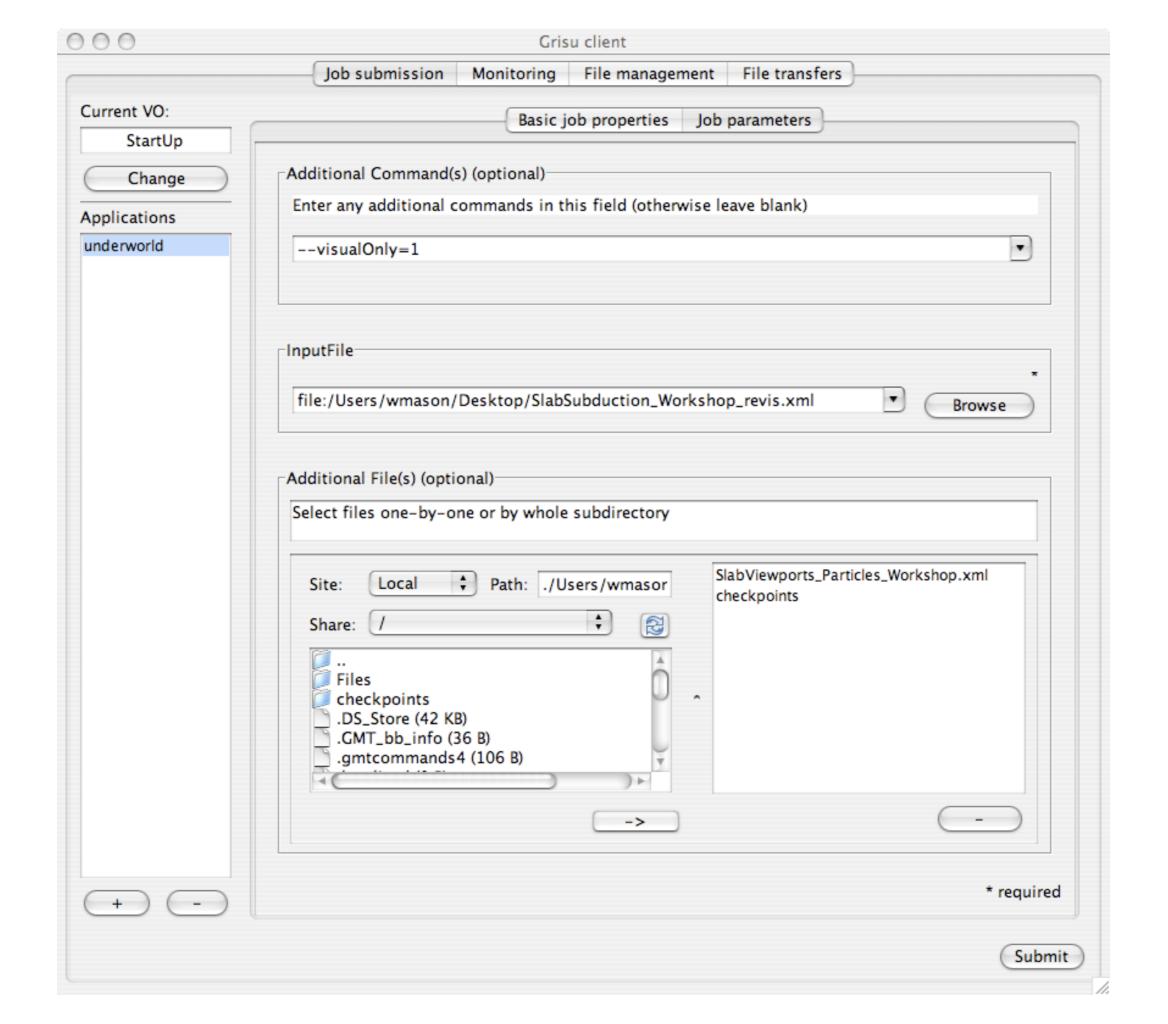






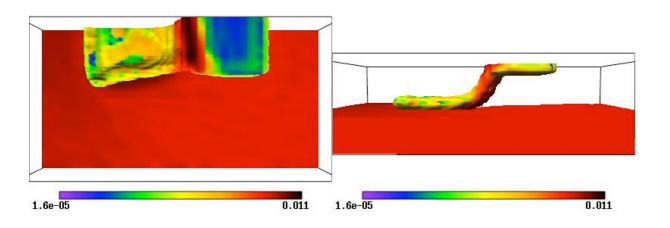




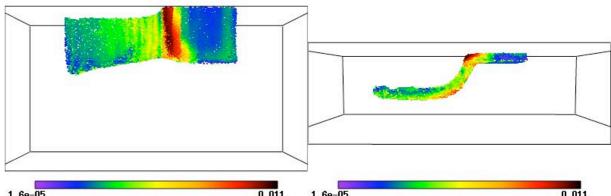


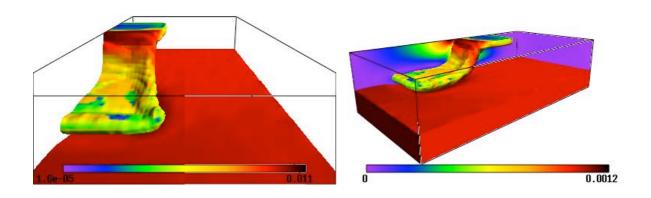
#4: SLABSUBDUCTION_WORKSHOP.XML

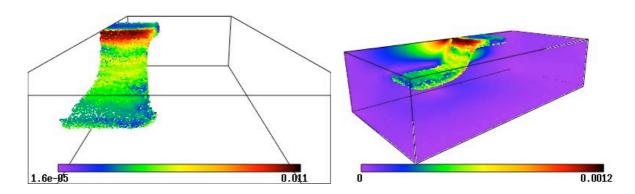
Template visualisation:



Example revisualisation:







- SlabViewports.xml
- slab isosurface draped in logscale of strain-rate invariant
- isosurface of lower mantle in red

- SlabViewports_Particles_Workshop.xml
- slab particles plotted in logscale of strain-rate invariant











Underworld Module Installations

- List of Underworld module installations (ARCS & NCI NF sites)
 - http://nf.nci.org.au/facilities/software/software.php?
 software=Underworld&all_sites=yes







- older modules in this list are no longer grid-enabled (only 1.2.0)
- Monash Sun Grid (MSG)



- currently Monash access only (command-line)
- Monash is looking into connecting the MSG to the ARCS Grid
- http://www.monash.edu.au/eresearch/services/mcg/msg.html











Underworld Module Installations

- Underworld module installations are planned for additional sites
- If there is no Underworld module installed on a cluster on the Grid that you want to use / already have access to, please let AuScope know (underworld-users@vpac.org) - we'll get one installed & grid-enabled for you
- List of ARCS sites / High Performance Computing (HPC) facilities:
 - http://www.arcs.org.au/products-services/systems-services/ compute-services/hpc-facilities











ARCS IDP & SERVICES

- You have been using the ARCS IdP
- Institutional IdPs will be available in coming months, including Monash University
 - will mean you can login to Grisu & other ARCS Services using your insitutional username and password (e.g. authcate for Monash users)
 - ARCS and your new IdP can arrange for secure transfer of your auEduPersonSharedToken from the ARCS IdP to your new IdP
 - participating members listed at <u>https://www.federation.org.au/FedManager/listMembers.do</u>











VIRTUAL ORGANISATIONS (VOS)

- Workshop VO will last until 19 June 2009
 - download, or copy today's output to your StartUp VO, before this date!
- StartUp VO only allows for 15 minute test jobs
- Each research group can have a Virtual Organisation (VO)
 - contact ARCS to create your group's VO
 - ask the relevant site to support your group's VO (cluster usage charges may apply)
 - e.g. the "MonashGeo" VO has been set up for the AuScope Underworld user community at Monash University to use VPAC cluster resources
- Users within a VO cannot see each other's data in Grisu (although still have access if the paths are known)
- Users can see and access each other's data using other GridFTP tools (e.g. Hermes)











OTHER FUTURE DEVELOPMENTS

- Next Underworld stable release & expanded user documentation
 - http://www.underworldproject.org
 - see http://www.underworldproject.org/documentation/
 UnderworldGridWorkshop2009.html for today's workshop slides
- Metascheduling
 - submit a compute job to the Grid (rather than a specific site), to run on the first available applicable resource
- ARCS Data Fabric (beta)
 - http://www.arcs.org.au/products-services/data-services
- Hear more about ARCS Systems tomorrow:
 - Jim McGovern, Systems Services Manager, ARCS: "ARCS Systems: from Grid to Cloud Computing", 10 to 11 am, Room 135, Building 26, Clayton Campus









